Akihide Kuwabara

List of Publications by Citations

154 papers	3,874 citations	34 h-index	56 g-index
171 ext. papers	4,526 ext. citations	5.3 avg, IF	5.35 L-index

#	Paper	IF	Citations
154	Structures and energetics of Ga2O3polymorphs. *Journal of Physics Condensed Matter*, **2007**, 19, 346211	1.8	182
153	Debye temperature and stiffness of carbon and boron nitride polymorphs from first principles calculations. *Physical Review B*, **2006**, 73,	3.3	181
152	First-principles approach to chemical diffusion of lithium atoms in a graphite intercalation compound. *Physical Review B*, **2008**, 78,	3.3	160
151	Accelerated Materials Design of Lithium Superionic Conductors Based on First-Principles Calculations and Machine Learning Algorithms. *Advanced Energy Materials*, **2013**, 3, 980-985	21.8	139
150	Why is sodium-intercalated graphite unstable?. *RSC Advances*, **2017**, 7, 36550-36554	3.7	129
149	First-principles calculations of lithium-ion migration at a coherent grain boundary in a cathode material, LiCoO(2). *Advanced Materials*, **2013**, 25, 618-22	24	118
148	Oxygen-vacancy ordering at surfaces of lithium manganese(III,IV) oxide spinel nanoparticles. *Angewandte Chemie - International Edition*, **2011**, 50, 3053-7	16.4	111
147	First-principles study of vacancy formation in hydroxyapatite. *Physical Review B*, **2007**, 75,	3.3	92
146	Pressure-induced phase transition in ZnO and ZnO□MgO pseudobinary system: A first-principles lattice dynamics study. *Physical Review B*, **2005**, 72,	3.3	91
145	Ab initio lattice dynamics and phase transformations of ZrO2. *Physical Review B*, **2005**, 71,	3.3	90
144	On the structural origin of the catalytic properties of inherently strained ultrasmall decahedral gold nanoparticles. *Nano Letters*, **2012**, 12, 2027-31	11.5	86
143	Effects of Off-Stoichiometry of LiC6 on the Lithium Diffusion Mechanism and Diffusivity by First Principles Calculations. *Journal of Physical Chemistry C*, **2010**, 114, 2375-2379	3.8	84
142	Crystalline Grain Interior Configuration Affects Lithium Migration Kinetics in Li-Rich Layered Oxide. *Nano Letters*, **2016**, 16, 2907-15	11.5	83
141	Lithium Atom and A-Site Vacancy Distributions in Lanthanum Lithium Titanate. *Chemistry of Materials*, **2013**, 25, 1607-1614	9.6	77
140	Prediction of ground-state structures and order-disorder phase transitions in II-III spinel oxides: A combined cluster-expansion method and first-principles study. *Physical Review B*, **2006**, 73,	3.3	72
139	Lattice dynamics and thermodynamical properties of silicon nitride polymorphs. *Physical Review B*, **2008**, 78,	3.3	71
138	First-principles study of bulk ordering and surface segregation in Pt-Rh binary alloys. *Physical Review B*, **2006**, 74,	3.3	65

137	Cubic and orthorhombic structures of aluminum hydride AlH3 predicted by a first-principles study. *Physical Review B*, **2005**, 71,	3.3	65
136	Dislocation-enhanced ionic conductivity of yttria-stabilized zirconia. *Applied Physics Letters*, **2003**, 82, 877-879	3.4	63
135	Chemical Expansion and Change in Lattice Constant of Y-Doped BaZrO3 by Hydration/Dehydration Reaction and Final Heat-Treating Temperature. *Journal of the American Ceramic Society*, **2013**, 96, 879-884	3.8	58
134	Domain boundaries and their influence on Li migration in solid-state electrolyte (La,Li)TiO3. *Journal of Power Sources*, **2015**, 276, 203-207	8.9	53
133	Ferroelectricity driven by twisting of silicate tetrahedral chains. *Angewandte Chemie - International Edition*, **2013**, 52, 8088-92	16.4	50
132	A combined conductivity and DFT study of protons in PbZrO3 and alkaline earth zirconate perovskites. *Solid State Ionics*, **2010**, 181, 130-137	3.3	49
131	Near-infrared analysis of protein secondary structure in aqueous solutions and freeze-dried solids. *Journal of Pharmaceutical Sciences*, **2006**, 95, 781-9	3.9	49
130	Machine-learning-based selective sampling procedure for identifying the low-energy region in a potential energy surface: A case study on proton conduction in oxides. *Physical Review B*, **2016**, 93,	3.3	47
129	First-principles calculations of lattice dynamics in CdTiO3 and CaTiO3: Phase stability and ferroelectricity. *Physical Review B*, **2011**, 84,	3.3	47
128	Domain boundary structures in lanthanum lithium titanates. *Journal of Materials Chemistry A*, **2014**, 2, 843-852	13	46
127	Chemical Pressure-Induced Anion Order-Disorder Transition in LnHO Enabled by Hydride Size Flexibility. *Journal of the American Chemical Society*, **2018**, 140, 11170-11173	16.4	43
126	First-principles study of cation disordering in MgAl2O4 spinel with cluster expansion and Monte Carlo simulation. *Physical Review B*, **2006**, 73,	3.3	42
125	Defect Chemistry of Rutile TiO2 from First Principles Calculations. *Journal of Physical Chemistry C*, **2013**, 117, 5919-5930	3.8	39
124	Ferroelectricity in wurtzite structure simple chalcogenide. *Applied Physics Letters*, **2014**, 104, 242909	3.4	36
123	First Principles Calculation of Defect Formation Energies in Sr- and Mg-Doped LaGaO3. *Journal of Physical Chemistry B*, **2004**, 108, 9168-9172	3.4	36
122	General rule for displacive phase transitions in perovskite compounds revisited by first principles calculations. *Physical Review Letters*, **2005**, 94, 035502	7.4	36
121	Geometric ferroelectricity in rare-earth compounds RGaO3 and RInO3. *Physical Review B*, **2009**, 79,	3.3	36
120	Oxygen loss and surface degradation during electrochemical cycling of lithium-ion battery cathode material LiMn2O4. *Journal of Materials Chemistry A*, **2019**, 7, 8845-8854	13	33

119	Cation ordering in A-site-deficient Li-ion conducting perovskites La(1□)/3LixNbO3. *Journal of Materials Chemistry A*, **2015**, 3, 3351-3359	13	30
118	The instability and resulting phase transition of cubic zirconia. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2001**, 312, 90-98	5.3	29
117	Hydride Conductivity in an Anion-Ordered Fluorite Structure LnHO with an Enlarged Bottleneck. *Chemistry of Materials*, **2019**, 31, 7360-7366	9.6	28
116	Ordering and segregation of a Cu75Pt25(111) surface: A first-principles cluster expansion study. *Physical Review B*, **2007**, 76,	3.3	28
115	Impact of lithium-ion ordering on surface electronic states of Li(x)CoO2. *Physical Review Letters*, **2013**, 111, 126104	7.4	27
114	First-Principles Calculations of Electronic Structure and Solution Energies of Mn-Doped BaTiO3. *Japanese Journal of Applied Physics*, **2010**, 49, 09MC01	1.4	26
113	Crystal and electronic structure changes during the charge-discharge process of Na4Co3(PO4)2P2O7. *Journal of Power Sources*, **2016**, 326, 220-225	8.9	25
112	Antiphase inversion domains in lithium cobaltite thin films deposited on single-crystal sapphire substrates. *Acta Materialia*, **2013**, 61, 7671-7678	8.4	24
111	Structural Distortion and Compositional Gradients Adjacent to Epitaxial LiMn2O4 Thin Film Interfaces. *Advanced Materials Interfaces*, **2014**, 1, 1400143	4.6	24
110	Superplastic flow stress and electronic structure in yttria-stabilized tetragonal zirconia polycrystals doped with GeO2 and TiO2. *Acta Materialia*, **2004**, 52, 5563-5569	8.4	24
109	Effects of Dislocations on the Oxygen Ionic Conduction in Yttria Stabilized Zirconia. *Materials Transactions*, **2004**, 45, 2042-2047	1.3	24
108	The electric field induced ferroelectric phase transition of AgNbO3. *Journal of Applied Physics*, **2016** , 119, 064102	2.5	24
107	Local condensation around oxygen vacancies in t-LaNbO4 from first principles calculations. *Physical Chemistry Chemical Physics*, **2009**, 11, 5550-3	3.6	23
106	Exploring a potential energy surface by machine learning for characterizing atomic transport. *Physical Review B*, **2018**, 97,	3.3	22
105	ZnTaON: Stabilized High-Temperature LiNbO-type Structure. *Journal of the American Chemical Society*, **2016**, 138, 15950-15955	16.4	22
104	Epitaxial Growth of LiMn2O4 Thin Films by Chemical Solution Deposition for Multilayer Lithium-Ion Batteries. *Journal of Physical Chemistry C*, **2014**, 118, 19540-19547	3.8	22
103	Adsorption and Diffusion of Oxygen Atoms on a Pt(211) Stepped Surface. *Journal of Physical Chemistry C*, **2013**, 117, 9772-9778	3.8	22
102	First-principles calculations of migration energy of lithium ions in halides and chalcogenides. *Journal of Physical Chemistry B*, **2006**, 110, 8258-62	3.4	22

101	Quantitative Evaluation of Electrochemical Potential Windows of Electrolytes for Electric Double-Layer Capacitors Using Ab Initio Calculations. *Journal of the Electrochemical Society*, **2010**, 157, A696	3.9	21
100	Atomic level changes during capacity fade in highly oriented thin films of cathode material LiCoPO4. *Journal of Materials Chemistry A*, **2017**, 5, 9329-9338	13	20
99	Lattice dynamics and ferroelectric properties of the nitride perovskite LaWN3. *Physical Review B*, **2017**, 95,	3.3	20
98	Selective Hydride Occupation in BaVO3□Hx (0.3 □x □0.8) with Face- and Corner-Shared Octahedra. *Chemistry of Materials*, **2018**, 30, 1566-1574	9.6	20
97	Microscopic mechanism of biphasic interface relaxation in lithium iron phosphate after delithiation. *Nature Communications*, **2018**, 9, 2863	17.4	20
96	On Hydride Diffusion in Transition Metal Perovskite Oxyhydrides Investigated via Deuterium Exchange. *Chemistry of Materials*, **2017**, 29, 8187-8194	9.6	20
95	Structure and chemistry of grain boundaries in SiO2-doped TZP. *Science and Technology of Advanced Materials*, **2001**, 2, 411-424	7.1	20
94	Hydride-based antiperovskites with soft anionic sublattices as fast alkali ionic conductors. *Nature Communications*, **2021**, 12, 201	17.4	19
93	A density functional study of vacancy formation in grain boundaries of undoped □alumina. *Acta Materialia*, **2014**, 69, 365-371	8.4	18
92	First-Principles Calculations of Rare-Earth Dopants in BaTiO3. *Japanese Journal of Applied Physics*, **2009**, 48, 09KC03	1.4	18
91	Density functional study of the phase stability and Raman spectra of YbO, YbSiO and YbSiO under pressure. *Physical Chemistry Chemical Physics*, **2018**, 20, 16518-16527	3.6	18
90	Theoretical and experimental analysis for site preference of rare earth elements in BaTiO3. *Ceramics International*, **2012**, 38, S25-S28	5.1	17
89	Anisotropic Permittivity of Tetragonal BaTiO$_{3}$: A First-Principles Study. *Japanese Journal of Applied Physics*, **2011**, 50, 09NE02	1.4	16
88	Mechanism of polarization switching in wurtzite-structured zinc oxide thin films. *Applied Physics Letters*, **2016**, 109, 102903	3.4	16
87	Competing structural instabilities in Bi2SiO5. *Physical Review B*, **2018**, 98,	3.3	16
86	BaScHO: H Conductive Layered Oxyhydride with H Site Selectivity. *Inorganic Chemistry*, **2019**, 58, 4431-4436	5.6	15
85	Direct Measurement of Electronic Band Structures at Oxide Grain Boundaries. *Nano Letters*, **2020**, 20, 2530-2536	11.5	15
84	First-Principles Study of Point Defect Formation in AgNbO3. *Japanese Journal of Applied Physics*, **2013**, 52, 09KF08	1.4	15

83	Theoretical investigation to thermal equilibrium concentration of point defect through first-principles calculation. *Science and Technology of Advanced Materials*, **2007**, 8, 519-523	7.1	14
82	Effect of Chemical Bonding States on the Tensile Ductility in Glass-Doped TZP. *Materials Science Forum*, **2001**, 357-359, 399-404	0.4	14
81	Synthesis and H conductivity of a new oxyhydride BaYHO with anion-ordered rock-salt layers. *Chemical Communications*, **2020**, 56, 10373-10376	5.8	14
80	Heterovalent Pb-substitution in ferroelectric bismuth silicate Bi2SiO5. *Journal of Materials Chemistry C*, **2016**, 4, 3168-3174	7.1	13
79	Polarization fluctuations in the perovskite-structured ferroelectric AgNbO3. *Physical Review B*, **2018**, 97,	3.3	13
78	Photo-induced change of dielectric response in BaCoSiO4 stuffed tridymite. *Journal of Applied Physics*, **2014**, 115, 164103	2.5	13
77	In situ electron microscopy analysis of electrochemical Zn deposition onto an electrode. *Journal of Power Sources*, **2021**, 481, 228831	8.9	13
76	Defects at the (1 1 0) surface of rutile TiO2 from ab initio calculations. *International Journal of Hydrogen Energy*, **2012**, 37, 8110-8117	6.7	12
75	Influence of Interaction between Neighboring Oxygen Ions on Phase Stability in Cubic Zirconia. *Journal of the American Ceramic Society*, **2002**, 85, 2557-2561	3.8	12
74	An Improved Method for Quantitatively Predicting the Electrochemical Stabilities of Organic Liquid Electrolytes Using Ab Initio Calculations. *Journal of the Electrochemical Society*, **2014**, 161, G7-G14	3.9	11
73	Oxygen-Vacancy Ordering at Surfaces of Lithium Manganese(III,IV) Oxide Spinel Nanoparticles. *Angewandte Chemie*, **2011**, 123, 3109-3113	3.6	11
72	A High-Coincidence Twin Boundary in Lithium Battery Material LiCoO2. *Nanoscience and Nanotechnology Letters*, **2012**, 4, 165-168	0.8	11
71	The influence of charge ordering on the phase stability of spinel LiNi2O4. *RSC Advances*, **2012**, 2, 12940	3.7	10
70	Local structural arrangements around oxygen and hydrogen-related defects in proton conducting LaP3O9 investigated by first principles calculations. *International Journal of Hydrogen Energy*, **2012**, 37, 7995-8003	6.7	10
69	First-principles investigation of R2O3(ZnO)3 (R=Al, Ga, and In) in homologous series of compounds. *Journal of Solid State Chemistry*, **2008**, 181, 137-142	3.3	10
68	High temperature plastic flow and grain boundary chemistry in oxide ceramics. *Journal of Materials Science*, **2005**, 40, 3129-3135	4.3	10
67	Local Bonding States of Titanium and Germanium-doped Tetragonal Zirconia Polycrystal and Their Correlation to High Temperature Ductility. *Materials Transactions*, **2002**, 43, 2468-2472	1.3	10
66	Microscopic characterization of the C–F bonds in fluorine–graphite intercalation compounds. *Journal of Power Sources*, **2020**, 445, 227320	8.9	10

65	Core□Shell Double Doping of Zn and Ca on □Ga2O3 Photocatalysts for Remarkable Water Splitting. *ACS Catalysis*, **2021**, 11, 1911-1919	13.1	10
64	Impact of local strain on Ti-L□□electron energy-loss near-edge structures of BaTiO□a first-principles multiplet study. *Microscopy (Oxford, England)*, **2014**, 63, 249-54	1.3	9
63	A First-Principles Study of the Ferroelectric Phase of AgNbO3. *Japanese Journal of Applied Physics*, **2012**, 51, 09LE02	1.4	9
62	Dopant arrangements in Y-doped BaZrO3 under processing conditions and their impact on proton conduction: a large-scale first-principles thermodynamics study. *Journal of Materials Chemistry A*, **2020**, 8, 12674-12686	13	8
61	Cr diffusion in □Al2O3: Secondary ion mass spectroscopy and first-principles study. *Physical Review B*, **2010**, 82,	3.3	8
60	Oxygen Affinity: The Missing Link Enabling Prediction of Proton Conductivities in Doped Barium Zirconates. *Chemistry of Materials*, **2020**, 32, 7292-7300	9.6	8
59	Theoretical and experimental studies of formation and migration of oxygen vacancies in BaMxTi1□O3(M = Zr, Ge). *Japanese Journal of Applied Physics*, **2016**, 55, 10TB02	1.4	7
58	Thermodynamics and structures of oxide crystals by a systematic set of first principles calculations. *Journal of Materials Chemistry*, **2010**, 20, 10335		7
57	Ab-initio multiplet calculation of oxygen vacancy effect on Ti-L2,3 electron energy loss near edge structures of BaTiO3. *Applied Physics Letters*, **2011**, 99, 233109	3.4	7
56	A First-Principles Study of the Ferroelectric Phase of AgNbO$_{3}$. *Japanese Journal of Applied Physics*, **2012**, 51, 09LE02	1.4	7
55	SYNTHESIS AND ELECTRICAL CONDUCTIVITY OF TETRA-VALENT CERIUM POLYPHOSPHATE BULKS. *Phosphorus Research Bulletin*, **2009**, 23, 20-24	0.3	7
54	Anion ordering enables fast H conduction at low temperatures. *Science Advances*, **2021**, 7,	14.3	7
53	Systematic analysis of electron energy-loss near-edge structures in Li-ion battery materials. *Physical Chemistry Chemical Physics*, **2018**, 20, 25052-25061	3.6	7
52	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO$_{3}$. *Japanese Journal of Applied Physics*, **2012**, 51, 09LE01	1.4	6
51	First-principles study of defect equilibria in lithium zinc nitride. *Journal of Physics Condensed Matter*, **2007**, 19, 046201	1.8	6
50	Grain Boundary Energy and Tensile Ductility in Superplastic Cation-doped TZP. *Materials Transactions*, **2004**, 45, 2144-2149	1.3	6
49	Responsive Four-Coordinate Iron(II) Nodes in FePd(CN). *Angewandte Chemie - International Edition*, **2020**, 59, 19254-19259	16.4	6
48	A computational search for wurtzite-structured ferroelectrics with low coercive voltages. *APL Materials*, **2020**, 8, 121102	5.7	5

47	Equilibrium hydrogen pressures in the V–H system from first principles. *International Journal of Hydrogen Energy*, **2019**, 44, 28909-28918	6.7	5
46	Negative-pressure-induced helimagnetism in ferromagnetic cubic perovskites Sr1−xBaxCoO3. *Physical Review Materials*, **2018**, 2,	3.2	5
45	First-Principles Calculations of Phase Transition in CaTiO3 under Negative Static Pressure. *Journal of the Korean Physical Society*, **2011**, 59, 2497-2502	0.6	5
44	Anisotropic Permittivity of Tetragonal BaTiO3: A First-Principles Study. *Japanese Journal of Applied Physics*, **2011**, 50, 09NE02	1.4	5
43	Ionic conduction mechanism in Ca-doped lanthanum oxychloride. *Dalton Transactions*, **2021**, 50, 151-156	4.3	5
42	High Rate Performance of Dual-Substituted LiFePO4 Based on Controlling Metastable Intermediate Phase. *ACS Applied Energy Materials*, **2018**, 1, 6736-6740	6.1	5
41	Application of machine learning-based selective sampling to determine BaZrO3 grain boundary structures. *Computational Materials Science*, **2019**, 164, 57-65	3.2	4
40	Isolated energy level in the band gap of Yb2Si2O7 identified by electron energy-loss spectroscopy. *Physical Review B*, **2016**, 93,	3.3	4
39	Quantitative analysis of Li distributions in battery material Li1-xFePO4 using Fe M2,3-edge and valence electron energy loss spectra. *Journal of Electron Microscopy*, **2017**, 66, 254-260		4
38	Variable anisotropy of ionic conduction in lithium nitride: Effect of duplex-charge transfer. *Physical Review B*, **2009**, 80,	3.3	4
37	First Principles Calculation of CO and H2 Adsorption on Strained Pt Surface. *Materials Transactions*, **2008**, 49, 2484-2490	1.3	4
36	Dehydration of Electrochemically Protonated Oxide: SrCoO with Square Spin Tubes. *Journal of the American Chemical Society*, **2021**, 143, 17517-17525	16.4	4
35	Transition-Metal Distribution in Brownmillerite CaFeCoO. *Inorganic Chemistry*, **2019**, 58, 10209-10216	5.1	3
34	A Density Functional Study of Oxygen Adatoms on a Step-Doubled Platinum Surface. *Journal of Physical Chemistry C*, **2014**, 118, 23675-23681	3.8	3
33	Systematic calculations of On (n = 1 to 6) polytypes of LiCoO2. *Physica Status Solidi - Rapid Research Letters*, **2014**, 8, 545-548	2.5	3
32	Magnetic Properties of Ni Alloys for Superconducting Wire Substrates: A First-Principles Study. *Japanese Journal of Applied Physics*, **2009**, 48, 083003	1.4	3
31	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. *Materials Transactions*, **2004**, 45, 2106-2111	1.3	3
30	Theoretical Analysis of Oxygen Vacancy Formation in Zr-Doped BaTiO3. *Japanese Journal of Applied Physics*, **2012**, 51, 09LE01	1.4	3

29	Atomic-Scale Analysis of Biphasic Boundaries in the Lithium-Ion Battery Cathode Material LiFePO4. *ACS Applied Energy Materials*, **2020**, 3, 8009-8016	6.1	3
28	Alkali-Rich Antiperovskite MFCh (M = Li, Na; Ch = S, Se, Te): The Role of Anions in Phase Stability and Ionic Transport. *Journal of the American Chemical Society*, **2021**, 143, 10668-10675	16.4	3
27	Effects of Nitrogen/Fluorine Codoping on Photocatalytic Rutile TiO Crystal Studied by First-Principles Calculations. *Inorganic Chemistry*, **2021**, 60, 2381-2389	5.1	3
26	Theoretical investigation of solid solution states of Ti1−VxH2. *Acta Materialia*, **2017**, 134, 274-282	8.4	2
25	Surface design of alloy protection against CO-poisoning from first principles. *Journal of Physics Condensed Matter*, **2014**, 26, 355006	1.8	2
24	Effect of oxygen vacancy segregation in Au or Pt/oxide hetero-interfaces on electronic structures. *RSC Advances*, **2017**, 7, 36034-36037	3.7	2
23	First-Principles Calculations of Point Defect Formation and Anion Diffusion Mechanisms in the Oxyhydride Ba2ScHO3		2
22	In situ electron microscopic observation of electrochemical Li-intercalation into MoS2. *Solid State Ionics*, **2020**, 357, 115488	3.3	2
21	Structural phase transitions of LaScO3 from first principles. *Materials Today Communications*, **2021**, 26, 102048	2.5	2
20	First-Principles-Based Phonon Calculation and Raman Spectroscopy Measurement of RuGa2 and RuAl2 with High Thermoelectric Power Factors. *Materials Transactions*, **2016**, 57, 1050-1054	1.3	2
19	Flux Crystal Growth, Structure, and Optical Properties of the New Germanium Oxysulfide La4(GeS2O2)3. *Crystal Growth and Design*, **2020**, 20, 4054-4061	3.5	1
18	An alternative description of mass transfer through thick oxide films. *Scripta Materialia*, **2015**, 100, 66-69	3.6	1
17	Computer simulation of coherent BaZrO3/MgO interfaces. *Journal of the Ceramic Society of Japan*, **2011**, 119, 861-866	1	1
16	Superplastic Behavior in Small Amount of Ge-Ti Co-Doped TZP. *Materials Science Forum*, **2004**, 447-448, 365-372	0.4	1
15	Accelerated lithium ions diffusion at the interface between LiFePO4 electrode and electrolyte by surface-nitride treatment. *Solid State Ionics*, **2021**, 373, 115792	3.3	1
14	On-Chip Electrochemical Analysis Combined with Liquid-Phase Electron Microscopy of Zinc Deposition/Dissolution. *Journal of the Electrochemical Society*, **2021**, 168, 112511	3.9	1
13	Nanoscale Defluorination Mechanism and Solid Electrolyte Interphase of a MgF2 Anode in Fluoride-Shuttle Batteries. *ACS Applied Energy Materials*, **2021**, 4, 996-1003	6.1	1
12	First-principles study of the ferroelectric phase of AgNbO3 **2019**, 137-159		

11	Flux Crystal Growth, Crystal Structure, and Optical Properties of New Germanate Garnet CeCaMgGeO. *Frontiers in Chemistry*, **2020**, 8, 91	5
10	First-Principles Based Phonon Calculation and Raman Spectroscopy Measurement of RuGa2 and RuAl2 with High Thermoelectric Power Factor. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2015**, 79, 591-596	0.4
9	First Principles Calculations of Advanced Nitrides, Oxides and Alloys. *Key Engineering Materials*, **2008**, 403, 73-76	0.4
8	????????????????. *Electrochemistry*, **2007**, 75, 421-425	1.2
7	Criterion for High Temperature Failure and Grain Boundary Chemistry in Superplastic TZP. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2005**, 69, 835-840	0.4
6	Influence of Ag Clusters on the Electronic Structures of □GaO Photocatalyst Surfaces.. *ACS Omega*, **2021**, 6, 33701-33707	3.9
5	Ceramic Materials. Analysis of Phase Stability in Cubic Zirconia Solid Solutions by First Principle Molecular Orbital Method.. *Zairyo/Journal of the Society of Materials Science, Japan*, **2001**, 50, 619-624	0.1
4	Responsive Four-Coordinate Iron(II) Nodes in FePd(CN)4. *Angewandte Chemie*, **2020**, 132, 19416-19421	3.6
3	Hidden Ladder in SrMoO3/SrTiO3 Superlattices: Experiments and Theoretical Calculations. *Journal of the Physical Society of Japan*, **2020**, 89, 074801	1.5
2	Theoretical investigation of tetrahedral distortion of four-coordinate iron(II) centres in FePd(CN). *Dalton Transactions*, **2021**, 50, 1990-1994	4.3
1	Kinetic Control of Anion Stoichiometry in Hexagonal BaTiO3. *Inorganics*, **2022**, 10, 73	2.9